

Branched Polymers

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Abstract

Building on and from the work of Brydges and Imbrie, we give an elementary calculation of the volume of the space of branched polymers of order n in the plane and in 3-space. Our development reveals some more general identities, and allows exact random sampling. In particular we show that a random 3-dimensional branched polymer of order n has diameter of order \sqrt{n} .

1 Introduction

A **branched polymer of order n** in \mathbb{R}^d —or just “polymer” for short—is a connected set of n labeled unit spheres with nonoverlapping interiors. We will assume that the sphere labeled 1 is centered at the origin. See Figure 1 for an example in the plane.

Intended as a model in chemistry or biology, branched polymers are often modeled, in turn, by lattice animals (trees on a grid); see, e.g., [3, 5, 7, 10, 18, 19]. However, we will see that continuum polymers turn out to be in some respects more tractable.

The set of polymers can be parametrized locally by the spherical angles of the vectors connecting adjacent sphere centers. In these coordinates Brydges and Imbrie [2] showed that the space $B^d(n)$ of polymers of order n has total volume $(n-1)!(2\pi)^{n-1}$ for $d = 2$ and $n^{n-1}(2\pi)^{n-1}$ for $d = 3$. Their proof uses nonconstructive techniques such as equivariant cohomology and localization.

We give here an elementary proof, together with some generalizations and an algorithm for exact random sampling of polymers. In the planar case our algorithm has the added feature of being inductive, in the sense that a uniformly random polymer of order n is constructed from one of order $n-1$.

Although not explicit in their paper, the proof in [2] in fact shows that in the planar case the volume of the configuration space is unchanged when the radii of the individual disks are different. We use this fact in an essential way in our constructions.

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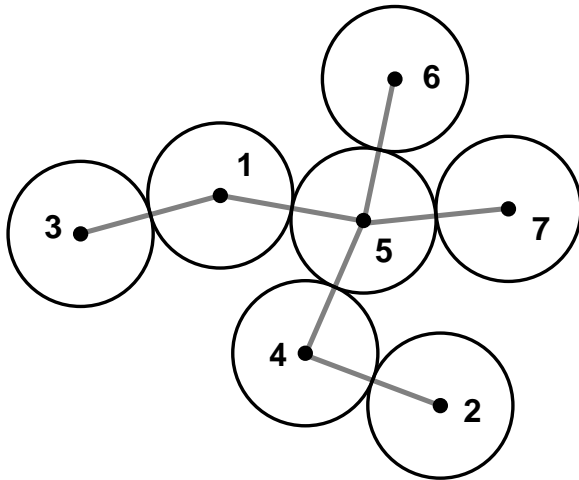


Figure 1: A branched polymer in the plane

2 The Planar Case

Let us observe first that $(n-1)!(2\pi)^{n-1}$ is also the volume of the space of “crossing worms”—that is, strings of labeled touching disks, beginning with disk 1 centered at the origin, but now with no constraint that disks may not overlap. See Figure 2 below for an example. Fixing the order of disks 2 through n in the crossing worm yields an ordinary unit-step walk in the plane of $n-1$ steps.

Yet another space of volume $(n-1)!(2\pi)^{n-1}$ is the space of “crossing inductive trees”, one of which is illustrated in Figure 3. A crossing inductive tree is a tree of n touching labeled disks with overlapping permitted, but required to satisfy the condition that for each $k < n$, disks $1, \dots, k$ must also form a tree. In other words, the vertex labels increase from the root 1. We will see that this space is in fact a certain limiting case of the space of polymers.

2.1 Coordinates

In the volume calculation we will need to consider polymers made of disks of arbitrary radius. Let $r_i \in (0, \infty)$ be the radius of the i th disk and $R = \{r_1, \dots, r_n\}$ be the vector of radii. Given a polymer $X = X(R)$, define a graph $G(X)$ with a vertex for each disk of X and an edge between vertices whenever the corresponding disks are adjacent. Almost surely $G(X)$ is a tree, that is, has no cycles. When $G(X)$ is a tree, we root $G(X)$ at the origin, and direct each edge away from the origin. This allows us to assign an “absolute” angle (taken counterclockwise relative to the X -axis) to each edge. Let e_1, \dots, e_{n-1} be the edges (chosen in some order) and $\theta_1, \dots, \theta_{n-1}$ the corresponding angles.

For a given combinatorial tree T , the set of polymers $X = X(R, T)$ with graph $G(X) = T$ can thus be identified with a subset of $[0, 2\pi)^{n-1}$. Call this set $\text{BP}_R(T)$. The boundary of $\text{BP}_R(T)$ corresponds to polymers having at least one cycle; the corresponding plane graphs $G(X)$ are obtained by adding one or more edges to T . Indeed, the boundary of $\text{BP}_R(T)$ is piecewise analytic and the pieces of codimension k correspond to polymers with k (facial) cycles.

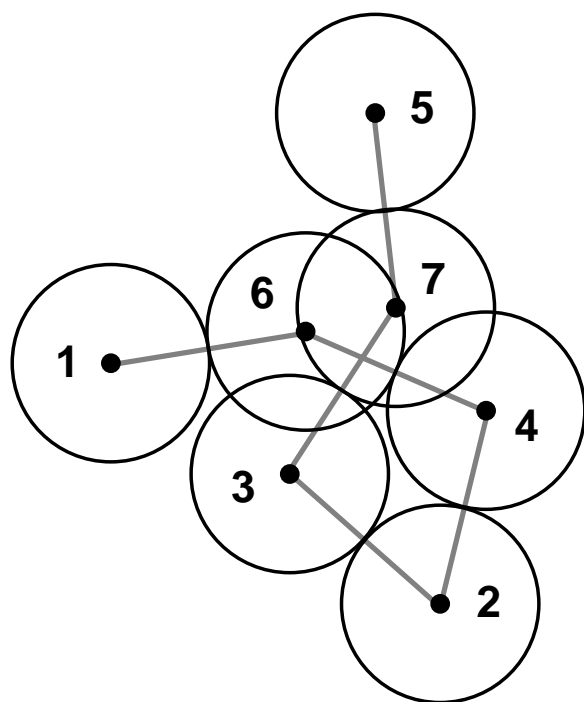


Figure 2: A crossing worm

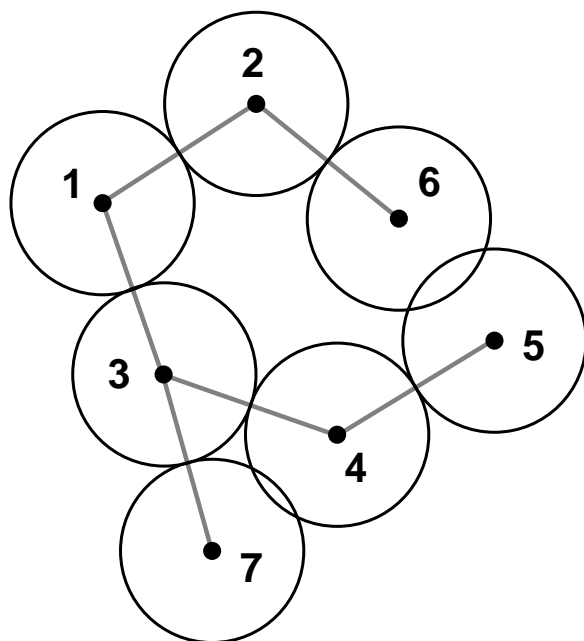


Figure 3: A crossing inductive tree

A polymer X with cycles lies in the boundary of each $\text{BP}_R(T)$ for which T is a spanning tree of the graph $G(X)$. Each such $\text{BP}_R(T)$ will contribute its own parameterization to X . Note, however, that some of the spanning trees may be unrealizable by unit disks (e.g. the star inside a 6-wheel); we just regard them as $\text{BP}_R(T)$ of zero volume.

We can construct a model for the parameter space of all polymers of size n and disk radii R by taking a copy of $\text{BP}_R(T)$ for each possible combinatorial type of tree, and identifying boundaries as above. Note that the identification maps are in general analytic maps on the angles: in a polygon with k vertices whose edges have fixed lengths r_1, \dots, r_k , any two consecutive angles are determined analytically by the remaining $k - 3$ angles.

2.2 Perturbations

A polygon P_m with m edges is determined up to rigid motion by $m-1$ consecutive edge lengths s_1, \dots, s_{m-1} and the $m-2$ consecutive interior angles $\phi_1, \dots, \phi_{m-2}$ with ϕ_i between edges s_i and s_{i+1} .

The space of perturbations of the angles of an m -gon P_m which preserve the edge lengths is $m-3$ -dimensional, and is generated by “local” perturbations which change only four consecutive angles. Here by perturbation we mean the derivative at 0 of a smooth one-parameter path in the space of m -gons with the same edge lengths as P_m . Such a perturbation is determined by the derivatives of the angles with respect to the parameter t along the path. We define $\frac{\partial}{\partial t_i}$ to be the infinitesimal perturbation of the angles of P_m , preserving the edge lengths, for which $\frac{\partial \phi_j}{\partial t_i} = 0$ unless j is one of $i-1, i, i+1, i+2$ (indices chosen cyclically) and $\frac{\partial \phi_i}{\partial t_i} = 1$. See Figure 4.

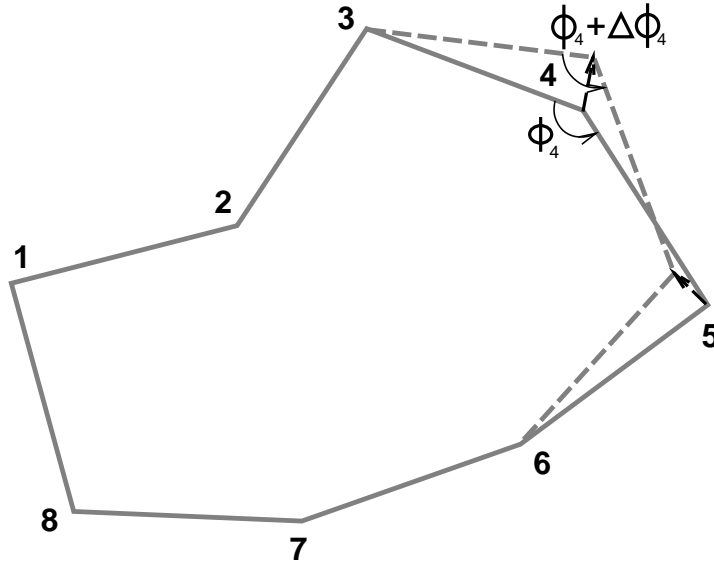


Figure 4: Local perturbation of vertex 4 of an octagon

For generic P , the $\frac{\partial}{\partial t_i}$ for $i = 1, 2, \dots, m-3$ generate all edge-length preserving perturbations of P . These $\frac{\partial}{\partial t_i}$ are useful because they provide a local infinitesimal coordinate charts

for the boundaries of the various sets $\text{BP}_R(T)$ which share the same cycle P_m .

For example, suppose that $\text{BP}_R(T)$ for some T is parametrized by angles $\theta_1, \dots, \theta_{n-1}$, and we are on a part of the boundary defined by a cycle with interior angles ϕ_1, \dots, ϕ_m (so the ϕ 's are differences of the θ 's). The infinitesimal (signed) volume of the part of the boundary swept out by the perturbations $\frac{\partial}{\partial t_i}$, for $i = 1, \dots, m-3$ is

$$(d\phi_1 \wedge \dots \wedge d\phi_{m-3}) \left(\frac{\partial}{\partial t_1}, \dots, \frac{\partial}{\partial t_{m-3}} \right) = \det \left(\frac{\partial \phi_i}{\partial t_j} \right)_{1 \leq i, j \leq m-3}. \quad (1)$$

That is to say, if $P(t_1, \dots, t_{m-3})$ for $(t_1, \dots, t_{m-3}) \in [0, \epsilon]^{m-3}$ is a perturbation of P_m , with $P(0, \dots, 0) = P_m$ and with $\frac{\partial P(0, \dots, 0)}{\partial t_i}$ having the above properties, then the signed volume swept out by all these perturbations, divided by ϵ^{m-3} , is given by (1).

We also need to consider perturbations of P_m which change the edge lengths. Let $\frac{\partial}{\partial S_i}$ be the perturbation in which two consecutive edge lengths increase and the rest remain unchanged, and only three angles change:

$$\begin{aligned} \frac{\partial s_i}{\partial S_i} &= \frac{\partial s_{i+1}}{\partial S_i} = 1 \text{ and } \frac{\partial s_j}{\partial S_i} = 0 \text{ for other } j, \text{ and} \\ \frac{\partial \phi_j}{\partial S_i} &= 0 \text{ unless } j = i-1, i \text{ or } i+1. \end{aligned}$$

This is obtained by moving only vertex i . Note that $\frac{\partial}{\partial S_i}$ for $i = 1, \dots, n$ generate all infinitesimal perturbations of the edge lengths. With the above $\frac{\partial}{\partial t_i}$, these $\frac{\partial}{\partial S_j}$ generate all motions of P_m .

2.3 Volumes

Here we determine how the volume of $\text{BP}_R(T)$ changes when one of the radii is increased.

Let X be an order- n polymer in the boundary of $\text{BP}_R(T)$. We assume that X is in a codimension-1 part of the boundary, that is, it has only one cycle, C , with vertices v_1, \dots, v_m in counterclockwise order. Let ϕ_1, \dots, ϕ_m be the corresponding interior angles of C . Let us assume that the tree T contains all edges of C except the edge between v_{m-1} and v_m , so that angles $\phi_1, \dots, \phi_{m-2}$ parametrize the polymers in $\text{BP}_R(T)$ close to X .

Recall that each edge of T is directed away from the root. Some of these are directed clockwise around C and some counterclockwise. Let v_i be the vertex of C closest to the root. The edges of C are oriented clockwise around C to the left of v_i and counterclockwise to the right of v_i . Let θ_{v_j} be the angle of the edge of T whose head is at v_j .

Lemma 1.

$$d\theta_{v_1} \wedge \dots \wedge \widehat{d\theta_{v_i}} \wedge \dots \wedge d\theta_{v_m} = (-1)^{m-2} d\phi_1 \wedge d\phi_2 \wedge \dots \wedge d\phi_{m-2} \wedge d\theta_{v_m}. \quad (2)$$

Proof. We can rewrite the left-hand side in terms of the $d\phi_j$ as follows. To the right of v_i , we have $\phi_j = \pi - (\theta_{v_{j+1}} - \theta_{v_j})$. To the left of v_i , we have $\phi_k = \pi + \theta_{v_{k-1}} - \theta_{v_k}$. Also, $\phi_i = \theta_{v_{i-1}} - \theta_{v_{i+1}}$. Replace successively $d\theta_{v_k}$ by $-d\phi_k$ for $k = 1, 2, \dots, i-1$. Then replace successively $d\theta_{v_\ell}$ by $-d\phi_{\ell-1}$ for $\ell = i+1, i+2, \dots, m-1$. There are precisely $m-2$ minus signs. \square

The volume form on $\text{BP}_R(T)$ is $d\theta_1 \wedge \cdots \wedge d\theta_{n-1}$. We can write this as $\alpha \wedge \beta$, where α is the form on the left-hand side of (2). The form β involves the edges which are not part of the cycle C .

If we fix the angles of a polymer X in the boundary of $\text{BP}_R(T)$ and change the radii by a small amount, from R to R' , the boundary of $\text{BP}_{R'}(T)$ moves in general away from X . To compute the change in volume of $\text{BP}_R(T)$, we integrate, along the entire codimension-1 boundary of $\text{BP}_R(T)$, this displacement times the volume form of the boundary. Let us consider a radius perturbation $\frac{\partial}{\partial S_i}$. On the boundary we use the local infinitesimal coordinates defined by the perturbations $\frac{\partial}{\partial t_i}$ for $i = 1, \dots, m-3$. The angles θ which are not part of the cycle C can be perturbed independently; let $\frac{\partial}{\partial \theta_j}$ be a perturbation of an angle θ_j not on C , which changes only this angle. The angle θ_m can also be perturbed independently of the angles ϕ_j in the cycle and other angles: it just determines the orientation of the cycle. Let $\frac{\partial}{\partial \theta_m}$ be a perturbation of θ_m . Let $\frac{\partial}{\partial \Theta}$ be the product of the perturbations for θ_m and the remaining angles not in C .

The local volume element gained or lost by $\text{BP}_R(T)$ is then the product of $\beta(\frac{\partial}{\partial \Theta})$ and

$$\omega = (d\phi_1 \wedge \cdots \wedge d\phi_{m-2}) \left(\frac{\partial}{\partial S_j}, \frac{\partial}{\partial t_1}, \dots, \frac{\partial}{\partial t_{m-3}} \right).$$

The total volume change of $\text{BP}_R(T)$ is the integral of ω times $\beta(\frac{\partial}{\partial \Theta})$ over the entire boundary of $\text{BP}_R(T)$. (More precisely, there is a corresponding form $\omega = \omega(C)$ for each codimension-1 piece of the boundary corresponding to the possible cycles C formed by T . The sum of the integrals of each form $\omega(C)$ times $\beta(\frac{\partial}{\partial \Theta})$ over the corresponding part of the boundary gives the total volume change.)

Now as T ranges over the trees obtained by removing one edge from C , the individual forms on the right-hand side of (2) are obtained from $d\phi_1 \wedge \cdots \wedge d\phi_m$ by removing two consecutive $d\phi_i$'s, and wedging the result with $d\theta_{v_m}$ (which, since it plays the role of a global rotation of the cycle, is the same for each i).

To prove that the sum of the volumes of the $\text{BP}_R(T)$ is constant, it suffices now to observe the following:

Lemma 2. *If $\phi_1 + \cdots + \phi_m$ is constant, then*

$$\sum_{i=1}^m d\phi_1 \wedge \cdots \wedge d\phi_{i-1} \wedge d\phi_{i+2} \wedge \cdots \wedge d\phi_m = 0$$

(with cyclic indices, and where if m is even we must put a $-$ sign in front of the last term $d\phi_2 \wedge \cdots \wedge d\phi_{m-1}$).

Proof. Substitute $d\phi_m = -d\phi_1 - \cdots - d\phi_{m-1}$ in each term and simplify. \square

It remains to show that this constant volume in fact takes the claimed value.

Theorem 3. *For any radius vector R of length n , the volume of the space of branched polymers is $(n-1)!(2\pi)^{n-1}$.*

Proof. Choose $\varepsilon > 0$ very small and let R be given by $r_i = \varepsilon^i$. Let X be a uniformly random configuration of disks with these radii, forming some labeled tree T . Suppose that for some $j < n$, disks 1 through j are connected. Then we claim that with probability near 1, disk $j+1$ touches one of disks 1 through j . To see this, observe that otherwise disk $j+1$ is connected to some previous disk i , $1 \leq i \leq j$, via a chain of (relatively) tiny disks whose indices all exceed $j+1$. Let disk k , $k > j+1$, be the one that touches disk $j+1$; then the angle of the vector from the center of disk k to the center of disk $j+1$ is constrained to a small range, else disk $j+1$ would overlap disk i . It follows that $BP_R(T)$ has lost almost an entire degree of freedom, thus has very small volume; in other words, the tree T is very unlikely.

Suppose, on the other hand, that for every j , disks 1 through j are connected. Then we may think of X as having been built by adding touching disks in index order, and since each is tiny compared to all previous disks, there is almost a full range 2π of angles available to it without danger of overlap.

It follows that as $\varepsilon \rightarrow 0$ the volume of the space of polymers with radius vector R approaches the volume of the space of crossing inductive trees, namely $(n-1)!(2\pi)^{n-1}$. Since this volume does not depend on R , we have equality. \square

2.4 Generalization to graphs

Let G be a graph on vertices $\{1, \dots, n\}$ whose edges are equipped with positive real lengths r_{ij} . A **G -polymer** is a configuration of points in the plane, also labeled by $\{1, \dots, n\}$, such that:

1. point number 1 is at the origin;
2. for each edge $\{i, j\}$ of G , the distance $\rho(i, j)$ between points i and j is at least r_{ij} ; and
3. the edges $\{i, j\}$ for which $\rho(i, j) = r_{ij}$ span G .

We denote the set of G -polymers realizing a given (spanning) tree T by $BP_G(T)$.

Note that if $R = (r_1, \dots, r_n)$, and G is the complete graph K_n with $r_{ij} = r_i + r_j$, then a G -polymer is precisely the set of centers of the disks of a polymer with radius vector R , in the sense of the previous sections. The volume V_G of the space of G -polymers is defined as before by the angles made by the vectors from i to j , where $\{i, j\}$ is an edge for which $\rho(i, j) = r_{ij}$.

In fact, the proof of Lemmas 1 and 2 extend without modification to show that V_G does not depend on the lengths r_{ij} (even if they fail to satisfy the triangle inequality), but only on the structure of G . This leaves us with the question of computing V_G for a simple graph G .

To do this, we label the edges of G arbitrarily as e_1, \dots, e_m and if $e_k = \{i, j\}$ we choose its edge-length r_{ij} to be ε^k for $\varepsilon > 0$ and very small. Then (since $\varepsilon \leq \frac{1}{2}$), for the volume of $BP_G(T)$ to be non-zero, there must not be an edge e_k of $G \setminus T$ such that k is the lowest index of all edges in the cycle made by adjoining e_k to T . If no such edge exists we say that T is “safe”; and in that case, arguing as in the proof of Theorem 3, there is almost no danger of violating condition (2) above in a random element of $BP_G(T)$. Thus the volume of the space of configurations in $BP_G(T)$ is nearly the full $(2\pi)^{n-1}$.

It follows that the volume of the space of *all* G -polymers is $\mu(G)(2\pi)^{n-1}$, where $\mu(G)$ is the number of safe spanning trees of G . Since $\mu(G)$ does not depend on the edge labeling, one might suspect that it has a symmetric definition, and indeed it does.

Lemma 4. *For any graph G , the number $\mu(G)$ of safe spanning trees of G is equal to the absolute value of the sum over all spanning subgraphs H of G , of $(-1)^{|H|}$.*

Proof. A simple inclusion-exclusion argument suffices. Let us fix any numbering of the edges of G and, for each spanning tree T , let $B(T)$ be the set of “bad” edges of $G \setminus T$, that is, edges which boast the lowest index of any edge in the cycle formed with T . Associate to each spanning graph H the spanning tree $T(H)$ obtained by repeatedly removing the lowest-indexed edge from each cycle. Then for n odd, a spanning tree T with set $B(T)$ of bad edges is counted once positively for each even subset of $B(T)$ and once negatively for each odd subset; and vice-versa for n even. It follows that in the sum (which we denote by $\mu(G)$) T has a net count of 0 unless $B(T)$ is empty, in which case it counts once positively (for n odd) or negatively (n even). But the trees for which $B(T)$ is empty are exactly the safe trees. \square

We conclude:

Theorem 5. *The volume of the space of G -polymers in the plane is $\mu(G)(2\pi)^{n-1}$.*

Comparing with Theorem 3, we have indirectly shown that $\mu(K_n) = (-1)^{n-1}(n-1)!$. In general $\mu(G) = |\mathcal{T}_G(0, 1)|$ where \mathcal{T}_G is the Tutte polynomial of G (see e.g. [1, 4, 17]). We note also that $\mu(G)$ plays the role of Brydges and Imbrie’s function “ J_C ” in the dimension-2 case.

The computation of $\mathcal{T}_G(0, 1)$, hence also of $\mu(G)$, is unfortunately #P-hard for general G [9]. The point $(0, 1)$ is not, however, in the region of the plane in which Goldberg and Jerrum [6] have recently shown the Tutte polynomial to be hard even to approximate. Thus, there is some hope that a “fully polynomial randomized approximation scheme” can be found for $\mu(G)$.

We conclude this section with a new solution of a notoriously difficult puzzle, which appears as an exercise in [14], derived from Rayleigh’s investigation (see [20]) of “random flight.” The exercise calls for proving the corollary below by developing the Fourier analysis of spherically symmetric functions, then deriving a certain identity involving Bessel functions. Curiously, it is (we believe) the only mention of *continuous* random walk in Spitzer’s entire book.

Corollary 6. *Let W be an n -step random walk in \mathbb{R}^2 , each step being an independent uniformly random unit vector. Then the probability that W ends within distance 1 of its starting point is $1/(n+1)$.*

Proof. The volume of the space of such walks, beginning from the origin, is of course $(2\pi)^n$. If the walk does *not* terminate inside the unit disk at the origin, it is in effect a C_{n+1} -polymer, where C_{n+1} is the $n+1$ cycle in which vertex i is adjacent to vertex $i+1$, modulo $n+1$. Since $\mu(C_{n+1}) = |1 - (n+1)| = n$, the volume of the space of C_{n+1} -polymers is $n(2\pi)^n$. Since the spanning tree with no edge between nodes 1 and $n+1$ is one of $n+1$ symmetric choices, the volume of the C_{n+1} -polymers which correspond to non-returning random walks is $n(2\pi)^n/(n+1)$, and the result follows. \square

2.5 The bipartite case

One special graph of interest is the complete bipartite graph $K_{m,n}$, representing particles of two types, each particle interacting only with particles of the other type. Note that in the hard-core model, phase transition has been proved in this situation [13]—in dimensions 2 and higher—but not for the complete graph.

Put $\mu_{m,n} = \mu(K_{m,n})$ and let $H(x, y)$ be the exponential generating function for $\mu_{m,n}$, given by

$$H(x, y) = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \mu_{m,n} \frac{x^m}{m!} \frac{y^n}{n!} .$$

Lemma 7.

$$H(x, y) = \log(e^{-x} + e^{-y} - e^{-x-y}) .$$

Proof. Observe that

$$\mu_{m,n} = \sum (-1)^k \mu(m_1, n_1) \mu(m_2, n_2) \dots \mu(m_k, n_k) C(m_1, \dots, m_k, n_1, \dots, n_k)$$

where the sum is over all partitions $m = m_1 + \dots + m_k$ and $n = n_1 + \dots + n_k$, and C is a combinatorial factor—the product of two multinomial coefficients divided by appropriate factorials when some of the pairs (m_i, n_i) are equal.

We claim that $dH(x, y)/dx = -1 + e^{-y-H(x,y)}$. This is because dH/dx in effect removes one vertex from the left (m -vertex) side of G ; this leaves singleton vertices from the right side, counted by e^y , and other components, counted by $e^{H(x,y)}$. The $-$ signs are contributed by edges connecting these components to the removed vertex, and the -1 summand comes about because there must be at least one remaining component.

Solving the differential equation with initial condition $H(0, y) = 0$ yields

$$H(x, y) = \log(e^{-x} + e^{-y} - e^{-x-y}) = -x - y + \log(e^x + e^y - 1) .$$

□

The argument generalizes to the complete k -partite case, giving

$$H(x_1, \dots, x_k) = -\sum_{i=1}^k x_i + \log \left(1 - k + \sum_{i=1}^k e^{x_i} \right) .$$

2.6 Construction

We now show inductively how to construct a uniformly random branched polymer of order n in the plane.

We begin with a unit disk centered at the origin. Suppose we have constructed a polymer of size $n-1$, $n > 1$. We choose a uniformly random disk from among the $n-1$ we have so far, then choose a uniformly random boundary point on that disk and start growing a new disk tangent to that point. If a disk of radius 1 fits at that point, this will define a polymer of size n .

Otherwise there is a radius $0 < r < 1$ at which a cycle forms with the new disk and some other disks present. At this point our polymer X is in the boundary of the space $\text{BP}_R(T)$, where $R = \{1, 1, \dots, 1, r\}$, and we need to choose some other tree T' for which X is in the boundary of $\text{BP}_R(T')$, and which has the property that increasing r (and leaving the angles fixed) will not cause the disks to overlap. There will be at least one possible such T' because the volume of $\text{BP}_R(T)$ is decreasing as r increases and so must be compensated by an increase in volume of some $\text{BP}_R(T')$. We choose randomly among the $\text{BP}_R(T')$ with increasing volume, with probability proportional to the infinitesimal change in the volumes of the $\text{BP}_R(T')$'s as r increases. This ensures that the volume lost to $\text{BP}_R(T)$ as r increases is distributed among the other $\text{BP}_R(T')$ so as to maintain the uniform measure. (In the language of Markov chains, this is the detailed balance condition).

Figure 5 shows snapshots of the construction of a random polymer, in the process of growing its third and fourth disks; Figure 6 shows a polymer of order 500 generated by this method.

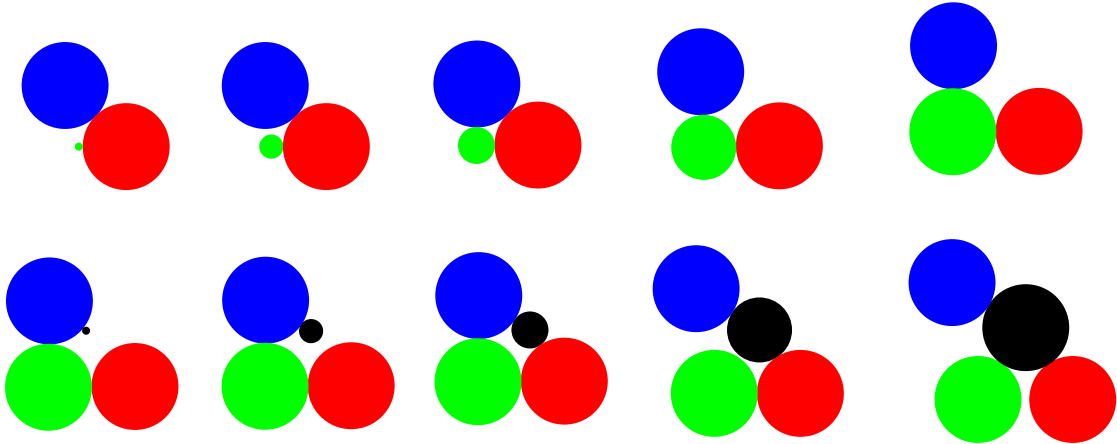


Figure 5: A random planar branched polymer growing new disks

All of the above is easily generalized to produce uniformly random G -polymers for any connected graph G with specified edge-lengths (and in fact we will need this construction later, when generating 3-dimensional polymers). The vertices of G may be taken in any order v_1, \dots, v_n having the property that the subgraph G_k induced by v_1, \dots, v_k is connected for all k . When a uniformly random G_{k-1} -polymer has been constructed, a new point corresponding to vertex v_k is added coincident to a point uniformly chosen from its neighborhood—in other words, we start by assuming that the edges of G_k incident to v_k are infinitesimal in length. These edges are then grown to their specified sizes, breaking cycles when they are formed in accordance with the rules above.

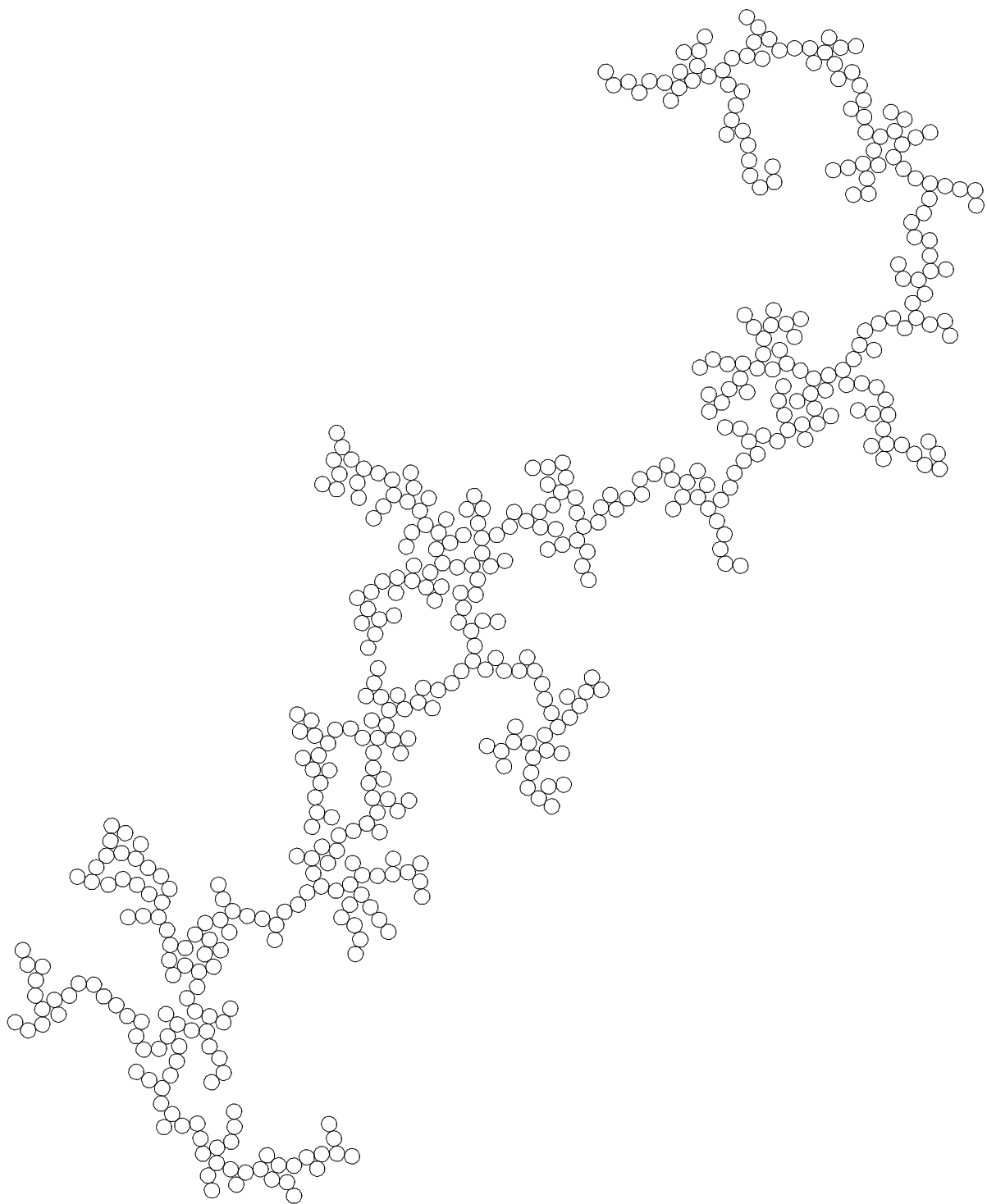


Figure 6: A uniformly random two-dimensional branched polymer of 500 disks.

3 The 3-dimensional Case

3.1 Volume invariance

Branched polymers in 3-space share many of the features of planar branched polymers. [2] showed that the volume of the configuration space of polymers in 3-space is $n^{n-1}(2\pi)^{n-1}$. Whereas the planar configuration space volume was independent of the radii of the balls, the same is not true in 3 dimensions. However, there is an invariance inherited from the plane under a different change of norm, which we now describe.

Let G be a graph with n vertices and edge weights $\beta_{ij} > 0$. A 3-dimensional G -polymer is a set of n points $v_1, \dots, v_n \in \mathbb{R}^3$ such that for all i, j we have

$$\|v_i - v_j\|^2 := (v_i^1 - v_j^1)^2 + \beta_{ij}((v_i^2 - v_j^2)^2 + (v_i^3 - v_j^3)^2) \geq 1,$$

with equality holding on a spanning tree of G .

When all β_{ij} are 1 this defines the standard branched polymer. Note that if $\|v_i - v_j\| = 1$ then v_j is on the surface of a spheroid centered at v_i . We measure the volume of the configuration space of 3-dimensional polymers using the normalized surface area of the corresponding spheroids; we will see that this volume is independent of the β_{ij} .

3.2 One-dimensional projections

Recall that the surface area measure of a sphere S^2 , projected to a line running through its center, projects to 2π times Lebesgue measure on the image segment. The same is true of the spheroid $\{v \in \mathbb{R}^3 : \|v\| = 1\}$ for any β , when projected to the x -axis, and it follows that for purposes of computing the volume of the configuration space, we may assume that the polymers are parametrized by the length of the projection of each $v_i - v_j$ on the x -axis together with its angle to the positive y -axis when projected onto the yz -plane.

Let x_1, \dots, x_n be the projections of v_1, \dots, v_n to the x -axis. We suppose, after relabeling if necessary, that the x_i are ordered $x_1 < x_2 < \dots < x_n$. If v_i and v_j are adjacent in the polymer then $|x_i - x_j| \leq 1$. (See Figure 7.)

Lemma 8. *Fix a graph G on $\{1, \dots, n\}$ with edge weights $\{\beta_{ij}\}$. The $n-1$ -dimensional volume of the set of G -polymers whose centers project to $x_1 < \dots < x_n$ is an integer multiple of $(2\pi)^{n-1}$ and depends only on the set of pairs i, j with $|x_j - x_i| > 1$.*

Proof. In any such polymer, the distance between the yz -plane projections of each pair i, j of adjacent centers is some fixed r_{ij} depending only on $|x_i - x_j|$ and β_{ij} . For non-adjacent centers, this distance is at least some r_{ij} provided $|x_i - x_j| \leq 1$; otherwise it is unconstrained.

It follows that if we let H be the graph on vertices $\{1, \dots, n\}$ given by $i \sim j$ iff $|x_i - x_j| \leq 1$, and define K to be the intersection of (the edges of) G and H (with edge-lengths supplied by G), then by Theorem 5 the desired volume is $\mu(K) \cdot (2\pi)^{n-1}$. \square

3.3 Complete graph

Note that H is a “unit interval graph” (see e.g. [12]) defined by overlapping unit-length intervals, in this case with their centers at the x_i . In the case of standard polymers, where

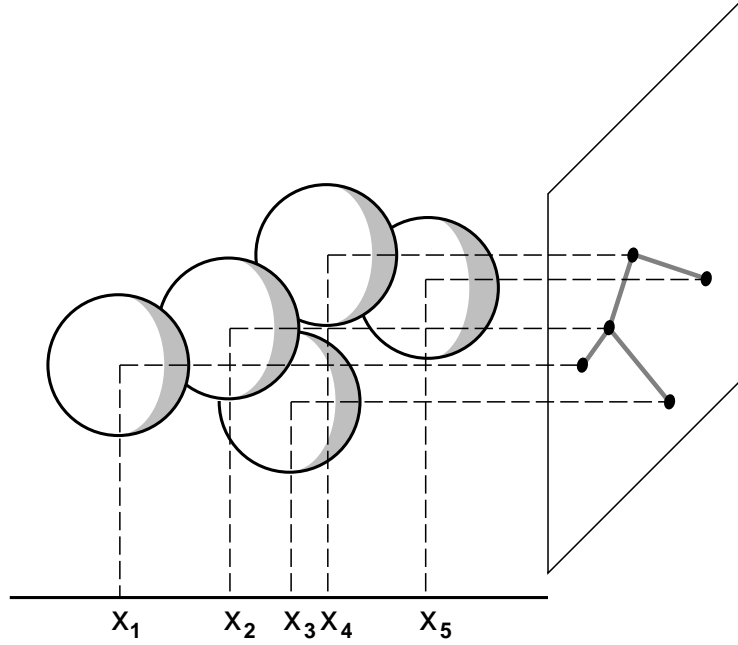


Figure 7: A branched polymer projected onto the x -axis and yz -plane.

G is complete, K is just H with appropriate edge lengths assigned. Thus $\mu(K) = \mu(H)$ and this is easy to compute: taking an arbitrary total order on the edges and $\beta_{e_k} = \epsilon^k$ for ϵ small (where e_k is the k th edge), the safe spanning trees of H are only those which are “inductive” in the sense of the Introduction: all paths from the root are increasing. It follows that each vertex $j > 1$ has as its parent some $i < j$ for which $x_i - x_j \leq 1$, thus

$$\mu(H) = \prod_{j=2}^n \gamma(j)$$

where $\gamma(j)$ is the number of $i < j$ for which $x_j - x_i \leq 1$.

It will be convenient temporarily to limit discussion to the space BP'_n of order- n polymers for which $x_1 = 0$, i.e. those whose roots extend farthest to the left along the x -axis. Define the *type* $\sigma(X)$ of a polymer X in BP'_n to be the permutation σ of $\{2, 3, \dots, n\}$ for which $x'_{\sigma(2)} < x'_{\sigma(3)} < \dots < x'_{\sigma(n)}$, where $x'_i := x_i \bmod 1$. Then $\mu(H)$ depends only on σ and we may call it $\mu(\sigma)$. The projections x_1, \dots, x_n are uniquely determined by σ and the arbitrary subset $\{x'_1, \dots, x'_n\}$ of $[0, 1]$, thus:

Corollary 9. *The volume of the space of branched polymers of type σ in BP'_n is precisely $\mu(\sigma)(2\pi)^{n-1}$.*

When σ is the identity permutation I , all the X_i are in $[0, 1]$, and μ takes its maximum value $(n-1)!$. This is just the planar case in disguise (although note that the three-dimensional volume of the polymers of type I incurs another factor of n on account of the choice of k for which $x_k = 0$). On the other end of the scale, the minimum value $\mu(\sigma) = 1$ is achieved in the spread-out case when $x_{i+2} - x_i > 1$ for each $i = 1, \dots, n-2$; the number of such σ is the “Euler number” E_{n-1} (see e.g. Stanley [15]).

Let T_n be a uniformly random tree on the labels $\{1, \dots, n\}$, with an independent uniformly random real length u_{ij} in $[0,1]$ assigned to each edge (i, j) . For each $j = 1, \dots, n$ let a_j be the sum of the lengths of the edges in the path from the root (vertex 1) to j in T ; and let $0 = b_1 \leq b_2 \leq \dots \leq b_n$ be the a_i taken in order. Let \mathbf{B} be the (random) vector $\langle b_1, \dots, b_n \rangle$.

Theorem 10. *Let X be a random branched polymer from BP'_n , and $0 = x_1 \leq x_2 \leq \dots \leq x_n$ the projections of its centers onto the x -axis. Then the random vector $\langle 0, x_2, x_3, \dots, x_n \rangle$ is distributed as \mathbf{B} .*

Proof. Suppose first that a tree T_n is fixed and that its \mathbf{B} -vector is of type σ . If we allow the edge-lengths of T_n to vary, we find that to maintain type σ the quantities $b_2 \bmod 1, \dots, b_n \bmod 1$, which are independent, uniformly random drawings from $[0,1]$, must fall in a particular order. Thus the probability that the edge-length assignments to any particular combinatorial tree T will yield a \mathbf{B} -vector of any fixed type σ is either 0 or a constant independent of T and σ .

In view of Corollary 9, it suffices then to show that the number of labeled trees T_n which contribute to type σ is $\mu(\sigma)$, but this is easy. Given \mathbf{B} , the node of T_n corresponding to b_j must have as its parent (counting node 1 as root) some node corresponding to an $i < j$ for which $b_j - b_i \leq 1$. \square

Theorem 10 says that the x -axis projections of a random $X \in BP'_n$ can be obtained by planting vertex 1 of T_n at $x = 0$ and stretching the tree to the right, letting the rest of its nodes mark the projections.

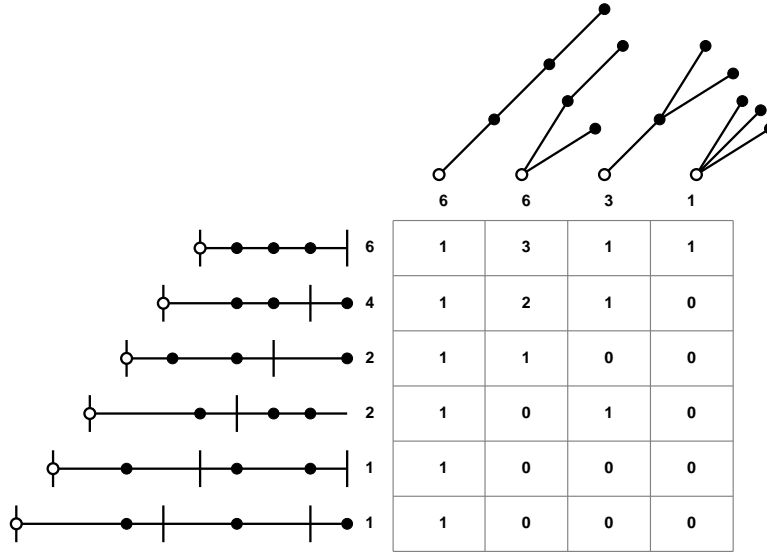


Figure 8: The matrix of types and trees for $n = 4$.

Figure 8 illustrates the case $n = 4$. The rows are indexed by types, presented as sample projections, each accompanied by its relative volume $\mu(\sigma)$. The columns are indexed by trees, each weighted by its number of distinct labelings (consistent with root at 1).

Note that the theorem does *not* say that the tree structure of a random 3-dimensional polymer is uniformly random; for example, no polymer can have a node of degree greater than 12. It does imply, however, when combined with the proof of Theorem 8, that if the polymer is not made of spheres but of ellipsoids with widely ranging $y - z$ axes, randomly assigned to labels, then indeed the tree structure approaches uniformly random labeled trees.

From Theorem 10 we can incidentally deduce the not completely obvious fact that the “reverse” vector $\langle 0, b_n - b_{n-1}, b_n - b_{n-2}, \dots, b_n \rangle$ has the same distribution as \mathbf{B} . For polymers, consequences of the theorem include the Brydges-Imbrie volume calculation and more:

Theorem 11. *The total volume of the space of 3-dimensional branched polymers of order n is $n^{n-1}(2\pi)^{n-1}$, and the expected diameter (combinatorial or Euclidean) of a random such polymer grows as $n^{1/2}$.*

Proof. For the volume, we apply Cayley’s theorem (to the effect that the number of labeled n -node trees is n^{n-2}) and the fact that, since relabeling of polymers preserves volume, the volume of BP'_n is just $1/n$ times the volume of the whole space.

For the diameter we make use of Szekeres’ Theorem (see [11, 16]) saying that the expected length of the longest path in a random tree on n labels is of order \sqrt{n} . The expected length of the longest path from the root in our edge-weighted tree T_n must therefore also be of order \sqrt{n} , and this is exactly the length of the projection of our random polymer on the x -axis. Since the space of polymers is independent of choice of axes, the spatial diameter of a random polymer must also be of order \sqrt{n} . \square

3.4 Construction

To construct a uniformly random three-dimensional branched polymer of order n , we first select a uniformly random labeled tree T , then a set $\{x_1, \dots, x_n\}$ of projected centers on the x -axis. We then build the yz -plane projection using our 2-dimensional polymer construction; this yields the locations of the n centers in 3-space, and it remains only to pick a root and translate it to the origin.

The tree T on vertices $\{1, \dots, n\}$ can be selected from the n^{n-2} possibilities by means of a Prüfer code (see, e.g., [8]), which is itself just a sequence of $n-2$ numbers between 1 and n . The first entry of the code is the label of the vertex adjacent to the least-labeled leaf of T ; that leaf is then deleted and succeeding entries defined similarly. The reverse process is also unique and easy.

The projections are defined by assigning independent uniformly random reals $u \in [0, 1]$ to each edge of T , then letting x_i be the length of the path from vertex i to vertex 1. The unit-interval graph H is defined as above on the tree-vertices, namely by $i \sim j$ if $|x_j - x_i| \leq 1$. Edge-lengths are assigned to H by $\ell(i, j) = \sqrt{1 - (x_j - x_i)^2}$ so that the spheres of the polymer corresponding to tree vertices i and j are touching just when their centers lie at distance $\ell(i, j)$ when projected onto the yz -plane, and in any case lie at least that far apart.

From the argument above we know that given x_1, \dots, x_n , the yz -plane projections are exactly a uniformly random planar H -polymer, which we then select using the methods of Section 2.6.

Combining the x -axis and yz -plane projections gives us the centers of a uniformly random branched polymer in 3-space (with spheres of diameter 1), except that sphere number 1 is

forced to have its center on the yz -plane; we now choose a sphere uniformly at random to be the new root, and translate the polymer so that this sphere's center is at the origin.

Figures 9, 10 and ?? are snapshots, from three angles, of a 3-dimensional branched polymer constructed as above.

4 Open problems

1. Is there a geometric interpretation of the local volume changes of the $BP_R(T)$ —which clearly depends on the shape of the cycle C ? This would lead to a possible natural geometrization of the space of polymers.
2. What are the volumes of $BP_R(T)$ for each T ?
3. What is the expected diameter (combinatorial or geometric) of a random two-dimensional branched polymer?
4. More generally, what do random polymers look like in the scaling limit, in any fixed dimension?

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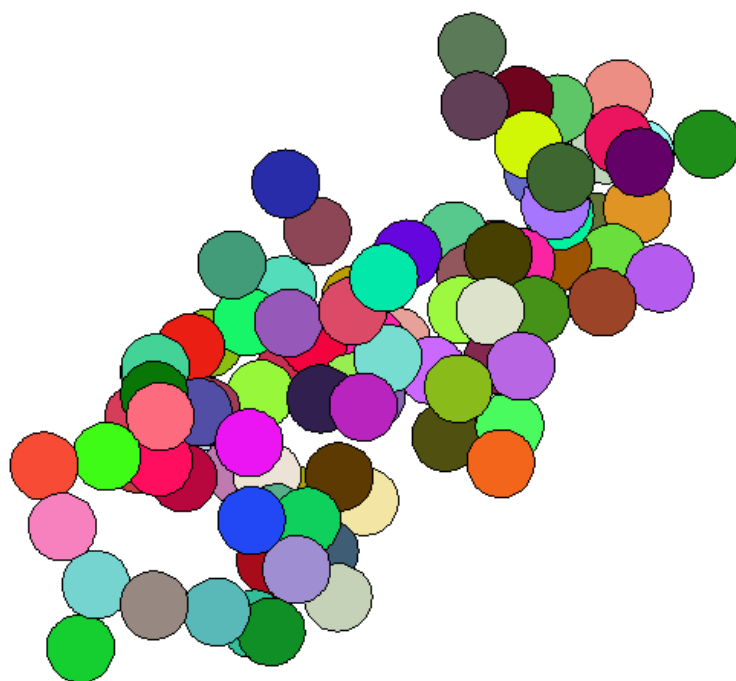


Figure 9: A random branched polymer in 3-space

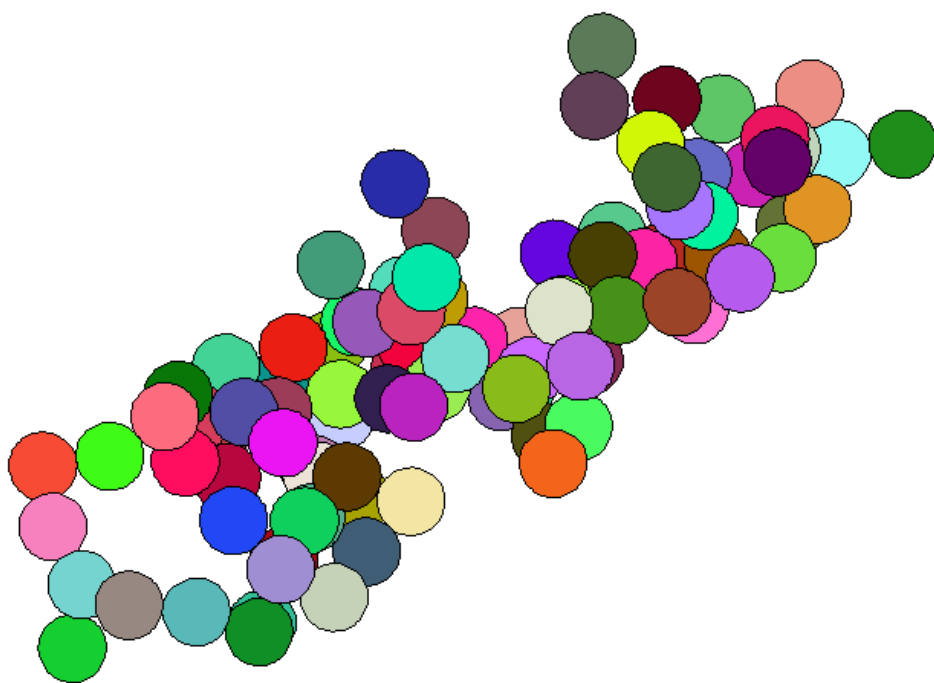


Figure 10: The same polymer, slightly rotated

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